

# First-principles description of disordered metallic systems with short-range order

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For many years the coherent potential approximation (CPA) has been widely used to describe the electronic structure of disordered systems. However, as a local mean-field theory of disorder, the CPA is unable to describe important environmental effects such as short-range order in alloys and spin fluctuations in magnets, amongst others. Only recently, the first satisfactory means of going beyond the CPA has been developed, the non-local coherent potential approximation (NLCPA),<sup>[1,2]</sup> which has also been derived within the first-principles Korringa-Kohn-Rostoker (KKR) multiple-scattering framework.<sup>[3]</sup> In this talk I describe the method and illustrate with KKR-NLCPA calculations for the effects of short-range order upon the electronic structure of alloys such as *CuZn* and *CuNi*.<sup>[4]</sup> I also discuss future applications such as transport properties, and developments such as combination with density functional theory for ab-initio calculations, which will enable effects such as charge correlations and lattice displacements to be taken into account self-consistently for the first time.

[1] M. Jarrell and H.R. Krishnamurthy, PRB 63, 125109 (2001)

[2] R. Moradian, B.L. Györffy, and J.F. Annett, PRL 89, 287002 (2002)

[3] D.A. Rowlands, J.B. Staunton, and B.L. Györffy, PRB 67, 115109 (2003)

[4] D.A. Rowlands, J.B. Staunton, B.L. Györffy, E. Bruno, B. Ginatempo (to be published)